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Formal Verification of a Floating-Point Expansion Renormalization Algorithm[★]

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Abstract. Many numerical problems require a higher computing precision than the one offered by standard floating-point formats. A common way of extending the precision is to use floating-point expansions. As the problems may be critical and as the algorithms used have very complex proofs (many sub-cases), a formal guarantee of correctness is a wish that can now be fulfilled, using interactive theorem proving. In this article we give a formal proof in Coq for one of the algorithms used as a basic brick when computing with floating-point expansions, the renormalization, which is usually applied after each operation. It is a critical step needed to ensure that the resulted expansion has the same property as the input one, and is more “compressed”. The formal proof uncovered several gaps in the pen-and-paper proof and gives the algorithm a very high level of guarantee.

Keywords: floating-point arithmetic, floating-point expansions, multiple-precision arithmetic, formal proof, Coq

1 Introduction

Many numerical problems require higher precisions than the standard *single*- (*binary32*) or *double*-precision (*binary64* [8]). Examples can be found in dynamical systems [1, 12], planetary orbit dynamics [14], computational geometry, etc. Several examples are given by Bailey and Borwein [2]. These calculations rely on arbitrary-precision libraries. A crucial design point of these libraries is the way numbers are represented. A first solution is the *multiple-digit* representation: each number is represented by one exponent and a sequence of possibly high-radix digits. The digits follow a regular pattern, which greatly facilitates the analysis of the associated arithmetic algorithms. GNU MPFR [6] is a C library that uses such a representation.

A second solution is the *multiple-term* representation in which a number is expressed as the unevaluated sum of several floating-point (FP) numbers. This

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sum is usually called a *FP expansion* (FPE). Since each term of this expansion has its own exponent, the term's positions can be quite irregular. The QD library [7] uses this approach and supports double-double and quad-double formats, i.e. numbers are represented as the sum of 2 or 4 double-precision FP numbers. Campary [11, 10] supports FPEs with an arbitrary number of terms, and also targets GPU implementation. Other libraries that manipulate FPEs are presented in [20, 17].

The intrinsic irregularity of FP expansions makes the design and proof of algorithms very difficult. Many algorithms are published without a proof, or with a proof so complex that is difficult to fully trust it. Obtaining formal proof of the critical parts of the algorithms that manipulate FPEs would bring much more confidence in them.

To make sure that a FPE carries enough information we need to ensure that it is *non-overlapping* (see Section 2). Even if the input FPEs satisfy this requirement, this property is often “broken” during the calculations, so after each operation we need to perform a *renormalization*. It is a basic brick for manipulating FPEs. While several renormalization algorithms have been proposed, until recently, Priest’s [12] was the only one provided with a complete correctness proof. However it uses many conditional branches, which makes it slow in practice. To overcome this problem, some of us developed in [10] a new algorithm (Alg. 3 below), that takes advantage of the machine pipeline and is provided with a correctness proof. However, the proof is complex, hence errors may have been left unnoticed. We decided to build a formal proof of that algorithm, using the Coq proof assistant and the Flocq library [5]. We also rely on a new iterator on lists that behaves better for functions that do not have an identity element [3]. There have already been some formal proofs on expansions [4]. Basic operations were formally proved in the PFF library (a library which preceded Flocq). The induction proofs were tedious, partly due to the formalization of FP numbers that was less convenient than that of Flocq.

The paper is organized as follows. Section 2 gives the pen-and-paper and the formal definitions of FPEs. Section 3 presents the renormalization algorithm and the wanted properties. Section 4 explains the formal verification of the various levels of the algorithm. Finally, Section 5 concludes this work.

2 Floating-point expansions

2.1 Pen-and-paper definitions

We begin with several literature definitions for FP expansions and their properties.

Definition 21 *A normal binary precision- p floating-point (FP) number has the form $x = M_x \cdot 2^{e_x - p + 1}$, with $2^{p-1} \leq |M_x| \leq 2^p - 1$. The integer e_x is the exponent of x , and $M_x \cdot 2^{-p+1}$ is the significand of x . We denote $\text{ulp}(x) = 2^{e_x - p + 1}$ (unit in the last place) [15, Chap. 2], and $\text{uls}(x) = \text{ulp}(x) \cdot 2^{z_x}$, where z_x is the number of trailing zeros at the end of M_x (unit in the last significant place).*

Definition 22 A FP expansion (FPE) u with n terms is the unevaluated sum of n FP numbers u_0, u_1, \dots, u_{n-1} , in which all nonzero terms are ordered by magnitude (i.e., if v is the sequence obtained by removing all zeros in the sequence u , and if sequence v contains m terms, $|v_i| \geq |v_{i+1}|$, for all $0 \leq i < m - 1$).

Arithmetics on FP expansions have been introduced by Priest [17], and later on by Shewchuk [20].

To make sure that an FPE carries enough information, it is required that the u_i 's do not “overlap”. The notion of *non-overlapping* varies depending on the authors. We give different definitions: \mathcal{P} -nonoverlapping and \mathcal{S} -nonoverlapping are common in the litterature. The third definition allows for a relatively relaxed handling of the FPEs and keeps the redundancy to a minimum. An FPE may contain interleaving zeros: the definitions that follow apply only to the non-zero terms of the expansion (i.e., the array v in Definition 22).

Definition 23 Assuming x and y are normal numbers with representations $M_x \cdot 2^{e_x - p + 1}$ and $M_y \cdot 2^{e_y - p + 1}$ (with $2^{p-1} \leq |M_x|, |M_y| \leq 2^p - 1$), they are \mathcal{P} -nonoverlapping (non-overlapping according to Priest's definition [18]) if $|e_y - e_x| \geq p$.

Definition 24 An expansion is \mathcal{P} -nonoverlapping if all its components are mutually \mathcal{P} -nonoverlapping.

Shewchuk [20] weakens this into:

Definition 25 An FPE u_0, u_1, \dots, u_{n-1} is \mathcal{S} -nonoverlapping (non-overlapping according to Shewchuk's definition [20]) if for all $0 < i < n$, we have $e_{u_{i-1}} - e_{u_i} \geq p - z_{u_{i-1}}$, i.e., $|u_i| < \text{ulp}(u_{i-1})$.

In general, a \mathcal{P} -nonoverlapping expansion carries more information than an \mathcal{S} -nonoverlapping one with the same number of components. Intuitively, the stronger the sense of the non-overlapping definition, the more difficult it is to guarantee it in the output. In practice, the \mathcal{P} -nonoverlapping property proved to be quite difficult to obtain and the \mathcal{S} -nonoverlapping is not strong enough, this is why we chose to compromise by using a different sense of non-overlapping, referred to as *ulp-nonoverlapping*, that we define below.

Definition 26 A FPE u_0, \dots, u_{n-1} is *ulp-nonoverlapping* if for all $0 < i < n$, $|u_i| \leq \text{ulp}(u_{i-1})$.

In other words, the components are either \mathcal{P} -nonoverlapping or they overlap by one bit, in which case the second component is a power of two.

Remark 27 Note that for \mathcal{P} -nonoverlapping expansions, we have $|u_i| \leq \frac{2^p - 1}{2^p} \text{ulp}(u_{i-1})$.

When using standard FP formats, the exponent range forces a constraint on the number of terms in a non-overlapping expansion. The largest expansion can be obtained when the largest term is close to overflow and the smallest is close

to underflow. When using Definition 24 or 26, the maximum expansion size is 39 for *double*-precision, and 12 for *single*-precision.

The algorithms performing arithmetic operations on FP expansions use the so-called *error-free transforms* (such as the algorithms 2Sum, Fast2Sum, Dekker’s product and 2MultFMA presented for instance in [15]), that make it possible to compute both the result and the error of a FP addition or multiplication. This implies that in general, each such algorithm, applied to two FP numbers, still returns two FP numbers.

In this article we make use of two algorithms that compute the exact sum of two FP numbers a and b and return the result under the form $s + e$, where s is the result rounded to nearest and e is the rounding error.

Algorithm 1 2Sum (a, b) .

```

 $s \leftarrow \text{RN}(a + b)$  // RN stands for performing the operation in rounding to nearest mode.
 $t \leftarrow \text{RN}(s - b)$ 
 $e \leftarrow \text{RN}(\text{RN}(a - t) + \text{RN}(b - \text{RN}(s - t)))$ 
return  $(s, e)$  such that  $s = \text{RN}(a + b)$  and  $s + e = a + b$ 

```

Algorithm 2 Fast2Sum (a, b) .

Input: exponent of a larger than or equal to exponent of b

```

 $s \leftarrow \text{RN}(a + b)$ 
 $z \leftarrow \text{RN}(s - a)$ 
 $e \leftarrow \text{RN}(b - z)$ 
return  $(s, e)$  such that  $s = \text{RN}(a + b)$  and  $s + e = a + b$ 

```

The *2Sum* (Algorithm 1) algorithm requires 6 *flops*, which it was proven to be optimal in [13], if we have no information on the ordering of a and b . However, if the ordering of the two inputs is known, a better alternative is *Fast2Sum* (Algorithm 2), that uses only 3 native FP operations. The latter one requires the exponent of a to be larger than or equal to that of b in order to return the correct result. This condition might be difficult to check, but of course, if $|a| \geq |b|$, it will be satisfied.

2.2 Coq definitions

We formalize FPEs as lists of real numbers with a property. We could have used arrays, but lists have an easy-to-use induction that was extensively used. This is not the data structure used for computing, but only for proving. As seen previously, FPEs are a bunch of FP numbers with some property (such as for instance $|u_i| \leq |u_{i-1}|$ or $|u_i| \leq \text{ulp}(u_{i-1})$). In a formal setting, we are trying to generalize this definition in order to cover many definitions, and have theorems powerful enough to handle both \mathcal{S} -nonoverlapping and \mathcal{P} -nonoverlapping FPEs for instance. The property between u_i and u_{i-1} will therefore be generic by default: it is a $P : \mathbb{R} \rightarrow \mathbb{R} \rightarrow \text{Prop}$, meaning a property linking two real numbers. This P will be \leq for ordered lists. For ulp-nonoverlapping, it is:

$$\text{fun } x \ y \Rightarrow |x| \leq \text{ulp}(y).$$

For \mathcal{S} -nonoverlapping, it is slightly more complex (see also Section 4.2):

$$\text{fun } x y \Rightarrow \exists e \in \mathbb{Z}, \exists n \in \mathbb{Z}, x = n \times 2^e \wedge |y| < 2^e.$$

We could have assumed that a FPE is a list where each value has this property with its successor (when it exists). Unfortunately, this fails when zeros appear in the FPE, therefore we have to account for the fact that we may have intermediate zeros inside our FPEs. This case was not considered in [10], so nothing was proved when a zero is involved. We get rid of this flaw and handle possible intermediate zeros in the proofs; in particular, we want to prove the FPE has the wanted property P , even if we remove the zeros. The Coq listing for defining a FPE with the P property is as follows:

```
Inductive Exp_P (P:R->R->Prop) : list R -> Prop :=
| Exp_Nil: Exp_P P List.nil
| Exp_One: forall x : R, Exp_P P (x :: nil)
| Exp_Z1: forall l: list R, Exp_P P l -> Exp_P P (0 :: l)
| Exp_Z2: forall x: R, forall l: list R, Exp_P P (x::l)
    -> Exp_P P (x :: (0 :: l))
| Exp_NZ: forall x y: R, forall l: list R,
    x <> 0 -> y <> 0
    -> Exp_P P (y::l)
    -> P x y -> Exp_P P (x :: (y :: l)).
```

Any empty or 1-element list is a FPE, and zeros in first or second position are useless. To prove that the list $x :: y :: l$ is a FPE, it suffices to prove that x and y are non-zero reals having the P property, and that $y :: l$ is a FPE. As common with formal developments, many lemmas need to be proved in order to use this definition (e.g., proving that a part of a FPE is also a FPE, or reversing a FPE). The most useful lemma is the one that proves that a given list is a FPE:

```
Lemma nth_Exp_P: forall (P:R->R->Prop) l,
  (forall i j, (0 <= i < length l)%nat
    -> (0 <= j < length l)%nat -> (i < j)%nat
    -> nth i l 0 <> 0 -> nth j l 0 <> 0
    -> P (nth i l 0) (nth j l 0))
  -> Exp_P P l.
```

where $\text{nth } i \ l \ 0$ is the i -th element of the list l or 0 if l is too short. This lemma means that if, whatever i and j such that $i < j$, and the i -th and j -th elements of the list are non-zero, and they have the P property, then the list is a FP expansion with the property P . The proof is straightforward, and it provides an easy way to handle intermediate zeros inside the formal verification of the algorithm. Let us now describe the renormalization algorithm published in [10], before describing its formal proof in Section 4.

3 Renormalization algorithm for FPEs

In [10] an algorithm with $m + 1$ levels that would render the result as an m -term \mathcal{P} -nonoverlapping FP expansion was presented. After test we concluded that using only ulp-nonoverlapping expansions greatly diminishes the cost of the algorithm while keeping the overlapping bits to a minimum, i.e., only one bit. This is why we only focus on the first two levels of the initial algorithm, that allow us to achieve the desired property.

Algorithm 3 Renormalization algorithm

Input: FP expansion $x = x_0 + \dots + x_{n-1}$ consisting of FP numbers that overlap by at most d digits, with $d \leq p - 2$; m length of output FP expansion.
Output: FP expansion $f = f_0 + \dots + f_{m-1}$ with $f_{i+1} \leq \text{ulp}(f_i)$, for all $0 \leq i < m - 1$.
1: $e[0 : n - 1] \leftarrow \text{VecSum}(x[0 : n - 1])$
2: $f[0 : m - 1] \leftarrow \text{VecSumErrBranch}(e[0 : n - 1], m)$
3: **return** FP expansion $f = f_0 + \dots + f_{m-2} + f_{m-1}$.

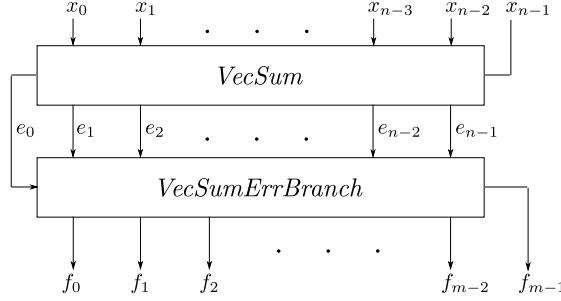


Fig. 1: Renormalization of n term-FPEs. The *VecSum* box performs Alg. 4 of Fig. 2, and the *VecSumErrBranch* box, Alg. 5 of Fig. 3.

The reduced renormalization algorithm (Algorithm 3, illustrated in Fig. 1) is made up with two different layers of chained *2Sum*. It receives as input an array with terms that overlap by at most d digits, with $d \leq p - 2$. Let us first define this concept.

Definition 31 Consider an array of FP numbers: x_0, x_1, \dots, x_{n-1} . According to Priest's [17] definition, they overlap by at most d digits ($0 \leq d < p$) if and only if $\forall i, 0 \leq i \leq n - 2, \exists k_i, \delta_i$ such that:

$$2^{k_i} \leq |x_i| < 2^{k_i+1}, \quad (1)$$

$$2^{k_i-\delta_i} \leq |x_{i+1}| \leq 2^{k_i-\delta_i+1}, \quad (2)$$

$$\delta_i \geq p - d, \quad (3)$$

$$\delta_i + \delta_{i+1} \geq p - z_{i-1}, \quad (4)$$

where z_{i-1} is the number of trailing zeros at the end of x_{i-1} and for $i = 0$, $z_{-1} := 0$.

It was proven in [10] that the algorithm returns an ulp-nonoverlapping expansion:

Proposition 32 *Consider an array x_0, x_1, \dots, x_{n-1} of FP numbers that overlap by at most $d \leq p - 2$ digits and let m be an input parameter, with $1 \leq m \leq n - 1$. Provided that no underflow / overflow occurs during the calculations, Algorithm 3 returns a “truncation” to m terms of an ulp-nonoverlapping FP expansion $f = f_0 + \dots + f_{n-1}$ such that $x_0 + \dots + x_{n-1} = f$.*

For the sake of simplicity, the 2 levels are represented as variations of the Algorithm *VecSum* of Ogita, Rump, and Oishi [20, 16], and treated separately. The proof was done using intermediate properties for each layer. Also, at each step it was proved that all the *2Sum* blocks can be replaced by *Fast2Sum* ones.

First level (line 1, Algorithm 3) The error-free transforms can be extended to work on several inputs by chaining, resulting in “distillation” algorithms [19]. The most frequently used one is *VecSum* (Fig. 2 and Algorithm 4). It is a chain of *2Sum* that performs an error-free transformation on n FP numbers.

Algorithm 4 *VecSum* (x_0, \dots, x_{n-1}) [20, 16].

Input: x_0, \dots, x_{n-1} FP numbers.

Output: $e_0 + \dots + e_{n-1} = x_0 + \dots + x_{n-1}$.

```

 $s_{n-1} \leftarrow x_{n-1}$ 
for  $i \leftarrow n - 2$  to 0 do
     $(s_i, e_{i+1}) \leftarrow 2Sum(x_i, s_{i+1})$ 
end for
 $e_0 \leftarrow s_0$ 
return  $e_0, \dots, e_{n-1}$ 

```

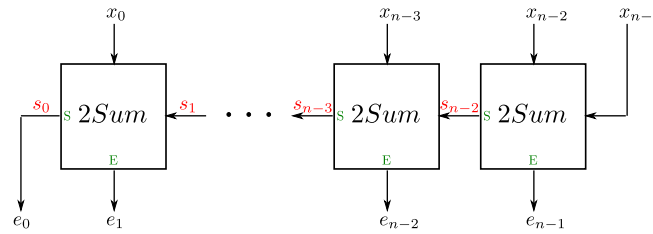


Fig. 2: *VecSum* with n terms. Each *2Sum* [15] box outputs the sum to the left and the error downwards.

The first level consists in applying Algorithm 4 on the input array, from where we obtain the array $e = (e_0, e_1, \dots, e_{n-1})$.

In [10] the following theorem was proved:

Proposition 33 *After applying the VecSum algorithm on an input array $x = (x_0, x_1, \dots, x_{n-1})$ of FP numbers that overlap by at most $d \leq p - 2$ digits, the output array $e = (e_0, e_1, \dots, e_{n-1})$ is \mathcal{S} -nonoverlapping and may contain interleaving zeros.*

Also, it was shown that for all arrays that satisfy the input requirements *2Sum* (6 FP operations) can be replaced by *Fast2Sum* (3 FP operations).

Second level (line 2, Algorithm 3) This level is applied on the array e obtained previously. This is also a chain of *2Sum*, but now we start from the most significant component. Also, instead of propagating the sums we propagate the errors. If however, the error after a *2Sum* block is zero, then we propagate the sum (this is shown in Figure 3). In what follows we will refer to this algorithm by *VecSumErrBranch* (see Algorithm 5).

Algorithm 5 *VecSumErrBranch* (e_0, \dots, e_{n-1})

Input: \mathcal{S} -nonoverlapping FP expansion $e = e_0 + \dots + e_{n-1}$; m length of the output expansion.

Output: FP expansion $f = f_0 + \dots + f_{m-1}$ with $f_{j+1} \leq \text{ulp}(f_j)$, $0 \leq j < m - 1$.

```

1:  $j \leftarrow 0$ 
2:  $\varepsilon_0 = e_0$ 
3: for  $i \leftarrow 0$  to  $n - 2$  do
4:    $(f_j, \varepsilon_{i+1}) \leftarrow 2Sum(\varepsilon_i, e_{i+1})$ 
5:   if  $\varepsilon_{i+1} \neq 0$  then
6:     if  $j \geq m - 1$  then
7:       return FP expansion  $f = f_0 + \dots + f_{m-1}$ .
8:     end if
9:      $j \leftarrow j + 1$ 
10:  else
11:     $\varepsilon_{i+1} \leftarrow f_j$ 
12:  end if
13: end for
14: if  $\varepsilon_{n-1} \neq 0$  and  $j < m$  then
15:    $f_j \leftarrow \varepsilon_{n-1}$ 
16: end if
17: return FP expansion  $f = f_0 + \dots + f_{m-1}$ .

```

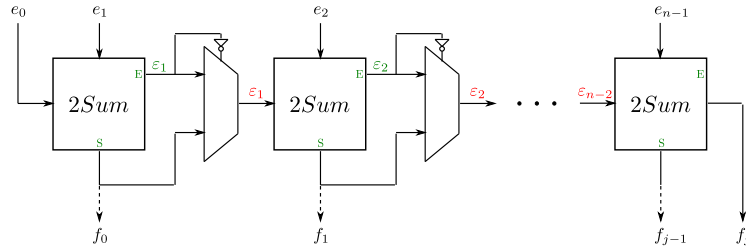


Fig. 3: *VecSumErrBranch* with n terms. Each *2Sum* box outputs the sum downwards and the error to the right. If the error is zero, the sum is propagated to the right.

For this algorithm we can also use *Fast2Sum* instead of *2Sum*. The following property holds:

Proposition 34 *Let e be an input array (e_0, \dots, e_{n-1}) of \mathcal{S} -nonoverlapping terms and $1 \leq m \leq n$ the required number of output terms. After applying `VecSumErrBranch`, the output array $f = (f_0, \dots, f_{m-1})$, with $0 \leq m \leq n - 1$ satisfies $|f_{i+1}| \leq \text{ulp}(f_i)$ for all $0 \leq i < m - 1$.*

Fig. 4 gives an intuitive drawing showing the different constraints between the FP numbers before and after the two levels of Algorithm 3. The notation is the same as in Fig. 1.

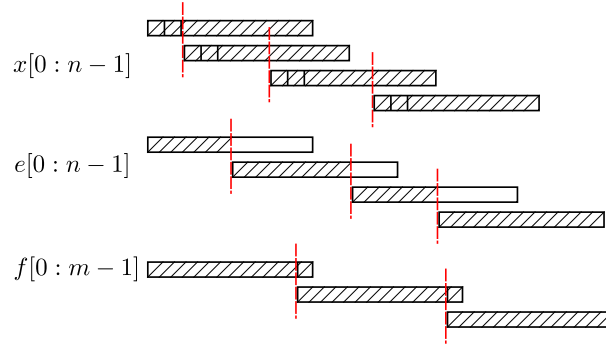


Fig. 4: The effect of Algorithm 3: x is the input FPE, e is the sequence obtained after the 1st level and f is the sequence obtained after the 2nd level.

Remark 35 *In the worst case, Algorithm 3 performs $n - 1$ `Fast2Sum` calls in the first level and $n - 2$ `Fast2Sum` calls plus $n - 1$ comparisons in the second one. This accounts for a total of $7n - 10$ FP operations.*

4 Formal proof

Let us now dive into what exactly is formally proved and how. We assume a FP format with radix 2 and precision p , that includes subnormals.

4.1 Prerequisites

A big difference between pen-and-paper proofs and formal proofs is the use of previous theorems. The proof in [10] relies on a result by Jeannerod and Rump [9] about an error bound on the sum of n FP numbers. In a formal proof, we need the previous result to be also formally proved (in the same proof assistant). As the Coq formal library of facts does not grow as fast as the pen-and-paper library of facts, we usually end up proving more results than expected, in particular, the result of Jeannerod and Rump does not belong to the Flocq library.

Theorem 41 (error_sum_n, from [9]) *Let l be a list of n FP numbers. Define $e = \sum_{i=0}^n l_i$ and $a = \sum_{i=0}^n |l_i|$. Let $f = \oplus_{i=0}^n l_i$ be the computed sum. Then $|f - e| \leq (n - 1)2^{-p}a$.*

The formal proof follows exactly the pen-and-paper proof from [9] without any problem. Note that the pen-and-paper result is more generic than the Coq one: it does not enforce the parenthesis, while we precisely choose where the parentheses are. As underflowing additions are correct, this holds even when subnormals are involved.

4.2 Formal proof of the first level

As explained in Section 3, Algorithm 3 has two steps. Let us deal with its first step, the *VecSum* algorithm (Algorithm 4).

Formalization of the *VecSum* algorithm A generic *VecSum_g* algorithm is defined. Indeed, *VecSum* is an iteration of a *2Sum* operator, where the sum is given to the next step, but we may imagine a *VecSum* with another operator, or with a *2Sum* operator, where the error is given to the next step (this is the case of the third step of the renormalization algorithm described in [10]). Many basic lemmas apply on all these examples and it is better to factorize them.

The Coq definition is a fixed-point operator applying on a list. The variant (for the termination) is *n*, that will be the length of the list *l*.

```
Fixpoint VecSum_g_aux (n:nat) (l:list R)
  {struct n} : list R := match n,l with
| 0, nil => nil
| 1, x :: nil => x :: nil
| S n, x :: y :: l =>
  (f x y) :: (VecSum_g_aux n (x+y-(f x y) :: l))
| _, _ => nil
end.

Fixpoint VecSum_g (l:list R) : list R
  := VecSum_g_aux (length l) l.
```

We prove various lemmas, including the fact that the output list has the same size as the input list and that the sum of the values of the input list is the same as the sum of the values of the output list.

Another point is that each value of the output list is exactly known from the input list (in the second level, we have tests that make this statement more complex). Taking the notations from Figure 2, the value e_0 (the last one computed) is the FP sum of all the x_i s. Using our formal definition, this means that the last element of the list is the iterated of the function $\text{fun } x \ y \Rightarrow x+y-(f \ x \ y)$. As for the i -th element, it is proved to be $f(s_{i+1}, x_{i+1})$, where x_k is the k -th element of the list and s_k is the iterated of the function $\text{fun } x \ y \Rightarrow x+y-(f \ x \ y)$ on the first k elements of the list. Note that lists are “numbered” from 0 to their size minus 1.

VecSum algorithm property Now let us deal with what is to be proved for this algorithm. In this case f will be the addition error function. We first look into the requirements on the input and output expansions. Let d be a positive integer such that $d \leq p - 2$, and the input an expansion with numbers that overlap by at most d digits. Formally, it is an expansion with a certain predicate IVS_P (for Input of *VecSum* Property). This property linking two reals x and y can be stated as follows: $|y| < 2^d \text{ulp}(x)$. As $d \leq p - 2$, it would intuitively mean that the expansion is clearly decreasing (as seen in Figure 4), but this is not the case when dealing with subnormal numbers. For instance, consider the smaller positive (subnormal) FP number η , then this property holds for η and himself, for η and 2η , and for 2η and η .

This is the reason why we choose:

$$IVS_P(x, y) = 2^{p-d} \text{ulp}(x) \leq \text{ulp}(y)$$

It is equivalent with the previous definition for normal numbers, but implies $|x| \leq |y|$, even when subnormals appear. Another interesting property is the fact that $IVS_P(x, y)$ implies that y is normal.

The output of the expansion is supposed to be \mathcal{S} -nonoverlapping (see Definition 25). We choose the simple definition:

$$OVS_P(x, y) := \exists e, n : \mathbb{Z}, y = n \cdot 2^e \wedge |x| < 2^e.$$

Said otherwise, there exists an exponent e such that y can be expressed with exponent e and $|x| < 2^e$. This e is an overestimation of the $\text{uls}(x)$ of Definition 24.

Proof of the *VecSum* algorithm property Here is some excerpt of the proof in [10]:

$$\begin{aligned} & |x_{j+1}| + |x_{j+2}| + \dots \leq \\ & \leq [2^d + 2^{2d-p} + 2^{3d-2p} + 2^{4d-3p} + \dots] \text{ulp}(x_j) \\ & \leq 2^d \cdot 2^p / (2^p - 1) \cdot \text{ulp}(x_j). \end{aligned}$$

This is partly wrong! In fact the geometric series should be bounded by:

$$2^d + 2^{2d-p} + 2^{3d-2p} + 2^{4d-3p} + \dots \leq 2^d / (1 - 2^{d-p}).$$

The proof can be fixed as the two inequalities were coarse enough, so there is no problem at this point.

A small gap in [10] is that it does not handle underflow. We did that in the formal proof without many problems. Given that the input list is an expansion with the IVS_P property, there can be at most one subnormal FP number (at the end). This implies a special treatment for one-element lists (which is not difficult) or lists with only one non-zero element (also not difficult) and taking care of the last element in all other cases. Furthermore, [10] proves that the output is non-overlapping assuming two successive outputs are non-zeros. Unfortunately, this does not cover the most complex case: a non-zero output

followed by one (or more) zero output, due to (partial) cancellation, and then another non-zero output. When considering the outputs, if e_i and e_{i+1} are non-zero, the corresponding s_i is bigger than s_{i+1} so that the exponent of s_i is bigger than that of s_{i+1} (property used in the proof in [10]). Yet, if e_i and e_{i+2} are non-zero, but $e_{i+1} = 0$, then the exponents of s_i and s_{i+2} may be in any order, and the proof does not hold anymore. We therefore needed several additional lemmas.

Lemma 42 *We assume we have an expansion $l = (x_i)$ with the IVS_P property with the length smaller than $2 + 2^{p-1}$. Then*

- Except if the $(x_k)_{k=i \text{ to } (n-1)}$ are all zeros, then $s_i \neq 0$.
- If $x_i \times s_{i+1} \geq 0$, then $\text{ulp}(s_{i+1}) \leq \text{ulp}(s_i)$.
- If $x_i \times s_{i+1} < 0$ and $|x_i| \leq 2|s_{i+1}|$, then $e_{i+1} = 0$.
- If $x_i \times s_{i+1} < 0$ and $2|s_{i+1}| < |x_i|$, then $\text{ulp}(s_{i+1}) \leq \text{ulp}(s_i)$.
- If $x_i \times s_{i+1} < 0$ and $|x_i| \leq 2|s_{i+1}|$, then $\text{ulp}(s_i) \leq \text{ulp}(s_{i+1})$.
- If $x_i \times s_{i+1} < 0$ and $|x_i| \leq 2|s_{i+1}|$ and $x_{i-1} \neq 0$, then $\text{ulp}(s_{i+2}) \leq \text{ulp}(s_i)$.

The lemma corresponds to various possibilities, including partial cancellation. The main result is then the following one:

Theorem 43 (incr_exp_sj) *Assuming an expansion $l = (x_i)$ with the IVS_P property, such that all $x_k \neq 0$, and such that its length is smaller than $2 + 2^{p-1}$. For all $i \leq j$ between 0 and the length of l , we have $\text{ulp}(s_i) \leq \max(\text{ulp}(s_j), \text{ulp}(s_{j+1}))$.*

In other words, if the exponent of s_j does not have the wanted property, then the exponent of s_{j+1} does. From this result, we deduce the main theorem of the *VecSum* algorithm:

Theorem 44 (VecSum_correct) *Assuming an expansion l with the IVS_P property and such that its length is smaller than $2 + 2^{p-1}$, then $\text{VecSum}(l)$ has the OVS_P property.*

To prove the OVS_P property, we just have to exhibit an exponent and prove its properties. Using the previous theorem, we exhibit the maximum between the exponents of s_j and s_{j+1} , and the rest of the proof is straightforward. There are special cases, e.g., small lists, or handling e_0 , which is not the same as the others e_i , or input lists with zeros. Yet, in the formal proof this is handled (with care) more easily than the exponent problem explained above. Note that we need a maximum size of the list: here $2 + 2^{p-1}$, meaning more than 4.5×10^{15} in *binary64* and more than 8 million in *binary32*. As done in [10], we also prove that a *Fast2Sum* can be used instead of a *2Sum* at every level of the algorithm.

4.3 Formal proof of the second level

Contrary to the formal proof of the first level, where we uncovered several difficulties, the formal proof of the second level was much simpler. Two additional features are the handling of subnormal numbers, which was trivial, and some discussions about the last two terms of the output list.

Formalization of the *VecSumErrBranch* algorithm As was done for *VecSum*, we define in Coq the formal version of *VecSumErrBranch*. It is more complicated and was therefore not put here. Refer to Figure 3 for a more understandable version. We proved several lemmas, including the fact that the sum of the values of the input list is the same as the sum of the values of the output list. We also prove that the output list has a smaller or equal size than the input list.

VecSumErrBranch algorithm property A difficulty is the need to reverse the list. *VecSum* was taking care of the values from the smallest to the largest, while *VecSumErrBranch* manipulates the values from the largest to the smallest. The input property of the expansion is the *OVS_P* property on the reverse list, meaning an expansion with the property

$$\text{fun } x \ y \Rightarrow \text{OVS_P}(y, x).$$

As for the output property, we only have the ulp-nonoverlapping property, with the definition

$$\text{OVSB_P}(x, y) := |y| \leq \text{ulp}(x).$$

Proof of the *VecSumErrBranch* algorithm property The input expansion has the *S*-nonoverlapping property, hence we can apply this lemma that will be helpful for our induction:

Lemma 45 *Let us assume that $(a :: b :: l)$ is an expansion with the *OVS_P*(y, x) property. Then*

- $(a + b :: l)$ is an expansion with the *OVS_P*(y, x) property.
- $(\circ(a + b) :: l)$ is an expansion with the *OVS_P*(y, x) property.
- $(a + b - \circ(a + b) :: l)$ is an expansion with the *OVS_P*(y, x) property.

Now we need to exhibit the first value output by *VecSumErrBranch*. It is the sum of several of the e_i s, in unknown number:

Lemma 46 *Let $l = (e_i)$ be an expansion with the *OVS_P*(y, x) property. We assume that it is non-empty and has no zeros. Define $x = e_0 \oplus \sum_{i=1}^n e_i$. There exists an integer n and a list l' such that:*

$$\begin{aligned} & \text{either } x \neq 0 \text{ or } (x = 0 \wedge l' \text{ is empty}) \\ & \text{and } \text{VecSumErrBranch}(l) = x :: l'. \end{aligned}$$

Note that the sum of $(e_i)_{1 \leq i \leq n}$ is exact. This is because e_i is kept to be propagated in the test when the error is zero, meaning the addition was exact.

All there is left to prove is that the *OVSB_P* (ulp-nonoverlapping) property is obtained with such terms:

Lemma 47 *Let us assume that $(b :: a :: l)$ is an expansion with the $OVS_P(y, x)$ property and that $b + a - b \oplus a \neq 0$. Let $l = (e_i)$. Then*

$$OVS_B_P \left(b \oplus a, \circ \left((b + a - b \oplus a) + \sum_{i=0}^n e_i \right) \right).$$

Then, we can prove the main theorem of the *VecSumErrBranch* algorithm:

Theorem 48 *Assume an expansion l with the $OVS_P(y, x)$ property. Then, $VecSumErrBranch(l)$ has the OVS_B_P property.*

As before, we take care of inputs with zeros using a special treatment. We also formally prove that the *Fast2Sum* operator can be used at every level.

A last point is that the output list is (nearly) non-zero. Due to the test, most output values cannot be zeros. All the $(f_i)_{i=0}$ to $j-2$ are non-zeros, but the last two terms f_{j-1} and f_j may be zeros. Note that f_j is zero if and only if the list is composed only of zeros.

5 Conclusion

The renormalization algorithm is a call to the previously-defined functions, and the proofs are successive calls to the previous proofs. Here is a final Coq excerpt for the renormalization algorithm formal verification.

```

1 Context { prec_gt_0_ : Prec_gt_0 p }.
2 Variable d:Z.
3 Hypothesis d_betw: (0 < d <= p-2)%Z.
4
5 Variable l: list R.
6 Hypothesis F1: Forall format l.
7 Hypothesis H1: InputVecSum d l.
8
9 Let res := VecSumErrBranch (rev (VecSum l)).
10
11 Lemma Renorm_1: Forall format res.
12 Lemma Renorm_2:
13     fold_right Rplus 0 l = fold_right Rplus 0 res.
14 Lemma Renorm_3: INR (length l) <= 2 + bpow (p - 1) ->
15     OutputVecSumErrBranch res.
```

The hypotheses are as follows: $p > 0$ (Line 1), $0 < d \leq p - 2$ (Lines 2-3). The input is a list of reals called l (Line 5). This list is a list of FP numbers (Line 6) and has the *IVS_P* property (Line 7).

The result of the renormalization is then **res** which is the application of *VecSumErrBranch* on the reverse of the application of *VecSum* to l (Line 9).

We then have the three proved lemmas. The first one says that the result is a list of FP numbers (Line 11), the second one says that the sum of the

values resulted is equal to the sum of the values of the input l (Line 12–13), and the third one is the expected property: it is an expansion with the *OVS_BP* property (*ulp-nonoverlapping*) (Line 14–16). This was fully proved in the Coq proof assistant within a few thousand lines:

spec	proof	file
74	497	AboutFP.v
200	1049	AboutLists.v
19	24	Renormalization.v
168	1162	VecSum1.v
93	975	VecSumErrBranch.v
554	3707	total

AboutFP includes the result of the error of FP addition from [9]. AboutLists includes results about parts of lists (such as n first elements, n last elements).

A missing part in the formal verification is the handling of overflow, as Flocq does not have an upper bound on the exponent range. It is not a real flaw, as an overflow would produce an infinity or a NaN at the end of the algorithm as only additions are involved.

This work was unexpectedly complicated: the formal verification was tedious due to many gaps, both expected (e.g., underflow) or unexpected (error in [10], handling of intermediate zeros that greatly modifies the proofs). More precisely about the intermediate zeros, let us assume that the result of the renormalization is $(y_0, y_1, y_2, 0, y_3, y_4, 0, y_5, 0, 0, 0)$ with the $y_i \neq 0$. Then the pen-and-paper theorem of [10] ensures that *OVS_P*(y_0, y_1), *OVS_P*(y_1, y_2), and *OVS_P*(y_3, y_4). Our theorem formally proved in Coq ensures that *OVS_P*(y_0, y_1), *OVS_P*(y_1, y_2), *OVS_P*(y_2, y_3), *OVS_P*(y_3, y_4), and *OVS_P*(y_4, y_5). Interleaving zeros may seem a triviality as zeros could easily be removed, except that this is costly as it involved testing each value. For this basic block, it is much more efficient to handle zeros inside the proof than to remove them in the algorithm.

We had some hope to be able to automate that kind of proofs, as many such algorithms exist in the literature, but this experiment has shown that, even from a detailed and reasonable pen-and-paper proof, much remains to be done to get a formal one. This paper shows that complex algorithms in FP arithmetic really need formal proofs: it is otherwise impossible to be certain that special cases have not been forgotten or overlooked in the pen-and-paper proof, as was the case here.

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